7/17/20 (1)
(Talk at UT Austin PJM group meeting)

Modelling microswimmers and active particles

The main actors: $\rho(x,t)$ density of ... something ($\rho \geq 0$)

$u(x,t)$ "drift" Could be a combination of flow and swimming (active particles)

$D(x,t)$ Diffusion coefficient. Symmetric tensor.

Fokker-Planck eq'n:

$$\partial_t \rho = -\nabla\cdot(u\rho - D\nabla\rho) =: \mathcal{L}\rho$$

$$= -\nabla\cdot f, \quad f = u\rho - D\nabla\rho = \text{"flux"}$$

$$\frac{d}{dt}\int_\Omega \rho\, dV = -\int_\Omega \nabla\cdot f\, dV = -\int_{\underset{\text{boundary}}{\partial\Omega}} f\cdot\hat{n}\, dS$$

flux through boundary

No "exits": $f\cdot\hat{n} = 0$ (or $\int_{\partial\Omega} f\cdot\hat{n}\, dS = 0$)

"no-flux BC" $\int_\Omega \rho\, dV = 1$ is preserved.

Common special cases: $u\cdot\hat{n}|_{\partial\Omega} = 0$ (no wall penetration)

$\nabla\cdot u = 0$ (incompressible)

When is $\rho = \text{const} = \frac{1}{|\Omega|}$ a solution? (uniform density)

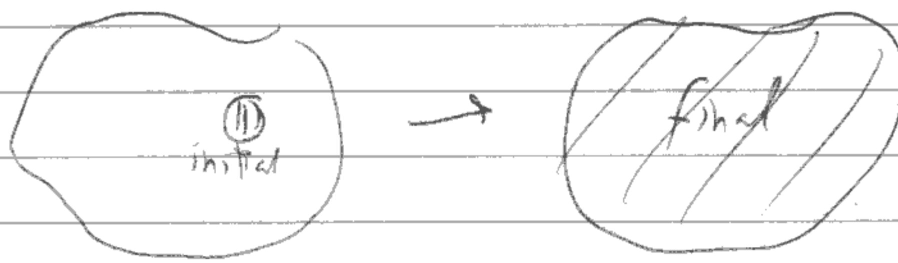
$|\Omega| =$ volume of Ω

$$\partial_t\left(\frac{1}{|\Omega|}\right) = 0 = -\nabla\cdot\left(u\frac{1}{|\Omega|} - D\nabla\left(\frac{1}{|\Omega|}\right)\right)$$

$$= -\frac{1}{|\Omega|}\nabla\cdot u \quad \text{So require } \nabla\cdot u = 0$$

<u>BUT</u>: BC is $n\cdot\left(u\frac{1}{|\Omega|} - D\nabla\left(\frac{1}{|\Omega|}\right)\right) = 0$ Also require $\hat{n}\cdot u\big|_{\partial\Omega} = 0$!

Both conditions are needed. The "~~invariant~~ uniform density" $\varphi = \frac{1}{|\Omega|}$ is the ultimate state.



Otherwise, φ is not constant in space, or even in time!

$$\frac{d}{dt}\int_\Omega f\log(f/g)\,dV = -D\int_\Omega f\left|\nabla\log(f/g)\right|^2 dV \leq 0$$

(Kullback-Leibler divergence)
or relative entropy

<u>Any</u> two initial conditions will converge to each other

"invariant density" $\cancel{\varphi(x,t) = \lim_{t_0\to-\infty}\int_\Omega p(x,t|x_0,t_0)}$

<u>Important</u>: this is true even when $u(x,t)$ depends on t! Very weak assumptions.

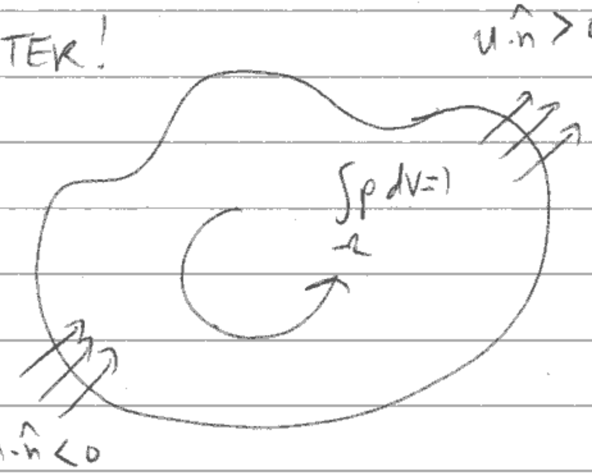
What does it mean to have $u \cdot \hat{n} \neq 0$ while still conserving total probability?

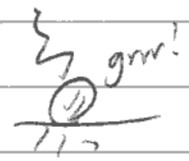
$\Rightarrow$ FILTER!

Fluid can get through, but particles can't

or

swimmer normal velocity doesn't vanish at wall





example: $\Omega = \{x > 0\}$

$$\frac{d}{dx}\left(u(x)\varphi - D(x)\varphi' \right) = 0, \qquad u(0)\varphi - D(0)\varphi'\Big|_{x=0} = 0$$

$$\varphi(\infty) = 0$$

$$\varphi(x) = C_1 \int_0^x \frac{u(\xi)}{D(\xi)}\, d\xi, \qquad x > 0$$

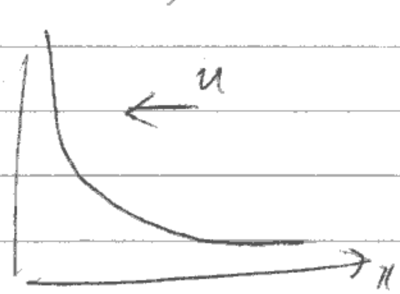
C_1 chosen so $\int_0^\infty \varphi \, dx = 1$

$u(\xi) = u = \text{const.} \quad (\nabla \cdot u = 0)$

$$\varphi(x) = -\frac{u}{D} e^{ux/D}, \qquad x > 0, \quad u < 0$$

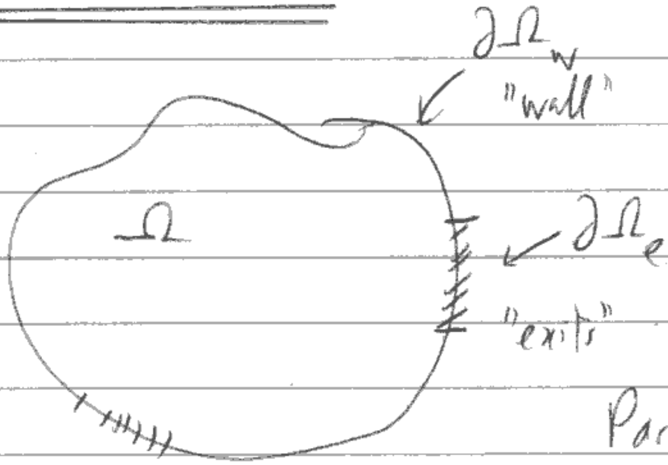
Particles accumulate at the wall.

The filter is working!



$u > 0$ not normalizable (∞ domain)

Walls and exits.



$$\partial\Omega = \partial\Omega_w \cup \partial\Omega_e$$

$$\hat{n}\cdot(u\rho - D\nabla\rho)\Big|_{\partial\Omega_w} = 0$$

$$\rho\Big|_{\partial\Omega_e} = 0$$

Particles "disappear" if they hit the exit.

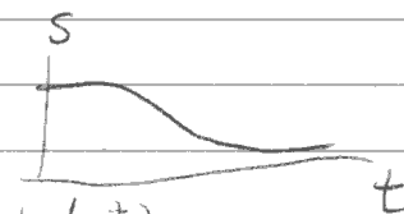
Same F-P equation as before.

$$\partial_t\rho = \mathcal{L}\rho = -\nabla\cdot(u\rho - D\nabla\rho), \quad \rho(x,t\,|\,x_0,t_0) = \delta(x-x_0)$$

Green's function

Survival probability:

$$S(t\,|\,x_0,t_0) = \int_\Omega \rho(x,t\,|\,x_0,t_0)\,dV$$



$$\partial_t S = -\int_{\partial\Omega} \underbrace{f}_{\text{flux}}\cdot\hat{n}\,dS \le 0.$$

(prob. density)

Define: $f(t\,|\,x_0,t_0) = -\dfrac{\partial S}{\partial t}$ pdf of first passage time.

$$\tau(x_0,t_0) = \int_{t_0}^{\infty}(t-t_0)\,f(t\,|\,x_0,t_0)\,dt$$

MEAN FIRST PASSAGE TIME or EXIT TIME (MET)

$$= -\int_{t_0}^{\infty}(t-t_0)\frac{\partial S}{\partial t}\,dt$$

by parts, throw out boundary term.

$$= \int_{t_0}^{\infty} S(t\,|\,x_0,t_0)\,dt$$

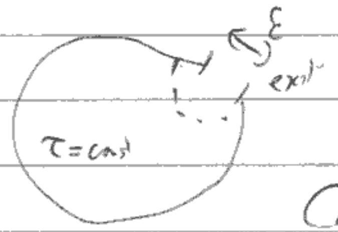
The most interesting property of the MET is that it satisfies its own equation:

$$-\partial_{t_0}\tau + \mathcal{L}_0^*\tau = 1$$

where $\mathcal{L}^*\tau = -u\cdot\nabla_0\tau - \nabla_0\cdot(D\nabla_0 f)$ is the <u>adjoint</u> of $\mathcal{L}$

This equation must be integrated backward in time
(Fun fact: no "terminal" condition.)

<u>Small exits:</u> the "narrow escape" problem.



: τ ~~becom~~ becomes constant over the domain, except boundary layer near the exit!

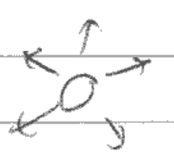
Can then do some nice asymptotics. $(u \equiv 0)$

$$\tau_{2D} \sim \frac{\cancel{}\,|\Omega|}{2\pi D}\log\varepsilon\,, \quad \tau_{3D} \sim \frac{\cancel{}\,|\Omega|}{4\pi D\varepsilon} \qquad \varepsilon\downarrow 0$$

2 or 1, depending on whether exit is at boundary

Current work: derive estimates for MET with drift.
(with Yu Feng)

$u \sim -\frac{A\varepsilon}{r^2}\hat{r} \qquad \tau \sim \frac{|\Omega|}{4\pi A\varepsilon}$



$\tau \sim$ exponentially long